

10/560039

Connecting via Winsock to STN

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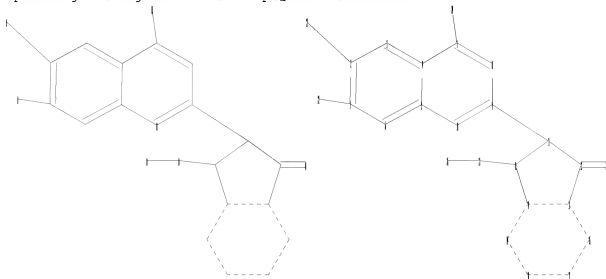
***** STN Columbus *****

FILE 'HOME' ENTERED AT 10:02:19 ON 11 FEB 2009

=> file reg

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Uploading C:\Program Files\Stnexp\Queries\11560039.str



chain nodes :

20 21 22 23 24 26

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19

chain bonds :

1-22 2-23 7-24 9-11 12-20 15-21 21-26

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10 11-15 11-12 12-13 13-14
13-16 14-15 14-19 16-17 17-18 18-19

exact/norm bonds :

11-15 11-12 12-13 12-20 13-14 13-16 14-15 14-19 15-21 16-17 17-18 18-19

exact bonds :

1-22 2-23 7-24 9-11 21-26

normalized bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10

isolated ring systems :

containing 1 :

10/560039

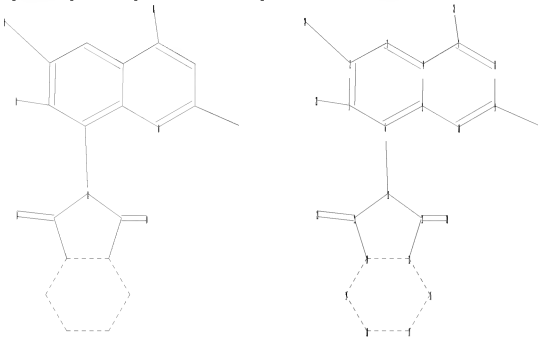
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 26:CLASS

L1 STRUCTURE UPLOADED

=>

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chain nodes :

20 21 22 23 24 25

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19

chain bonds :

1-23 2-24 6-11 7-25 9-22 12-20 15-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14
13-16 14-15 14-19 16-17 17-18 18-19

exact/norm bonds :

6-11 11-12 11-15 12-13 12-20 13-14 13-16 14-15 14-19 15-21 16-17 17-18
18-19

exact bonds :

1-23 2-24 7-25 9-22

normalized bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS

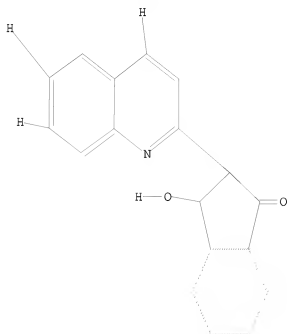
10/560039

L2 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

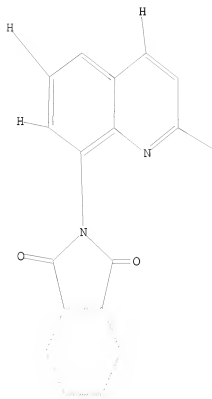


Structure attributes must be viewed using STN Express query preparation.

=> d 12

L2 HAS NO ANSWERS

L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 10:03:38 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 2343 TO ITERATE

100.0% PROCESSED 2343 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

L5

2 SEA SSS FUL L1

=> s l2 full

FULL SEARCH INITIATED 10:03:41 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 287 TO ITERATE

100.0% PROCESSED 287 ITERATIONS

12 ANSWERS

SEARCH TIME: 00.00.01

L6

12 SEA SSS FUL L2

=> file ca

=> s l5 or l6

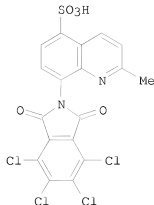
2 L5

L7 6 L6
8 L5 OR L6

=> d ibib abs fhistr 1-8

L7 ANSWER 1 OF 8 CA COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 142:58225 CA
TITLE: Use of quinaldine and naphthalene derivatives as crystallization modifiers for quinophthalone (and other) pigments.
INVENTOR(S): Stohr, Andreas; Schroeck, Manfred
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004108837	A1	20041216	WO 2004-EP6164	20040608
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10326631	A1	20050105	DE 2003-10326631	20030611
TW 258496	B	20060721	TW 2004-93113356	20040512
EP 1641885	A1	20060405	EP 2004-739693	20040608
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1806016	A	20060719	CN 2004-80016427	20040608
JP 2006527290	T	20061130	JP 2006-515849	20040608
US 20060150866	A1	20060713	US 2005-560039	20051208
PRIORITY APPLN. INFO.:			DE 2003-10326631	A 20030611
			WO 2004-EP6164	W 20040608
OTHER SOURCE(S):	MARPAT	142:58225		
GI				



AB Quinaldine and naphthalene derivs. are useful as crystallization modifiers in the

process of grinding and recrystn. of crude quinophthalone pigments from aqueous or/and organic solvent/water mixts. into fine-particle pigments.

Thus, I

(prepared by heating a mixture containing 100 g of phenol, 34 g of 8-aminoquinaldine-5-sulfonic acid and 49 g of tetrachlorophthalic anhydride 8 h at 180°, cooling to 90°, adding 300 mL of methanol, washing and drying at 40°) is used in recrystn. of crude quinophthalone pigment having particle size 2 cm (Pigment yellow 138) from xylene solution with additives of aliphatic amines.

IT 807657-04-1P

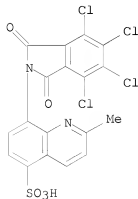
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(crystallization modifier; quinaldine and naphthalene derivs. as crystallization

modifiers in grinding and recrystn. of crude quinophthalone pigments)

RN 807657-04-1 CA

CN 5-Quinolinesulfonic acid, 2-methyl-8-(4,5,6,7-tetrachloro-1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)- (CA INDEX NAME)



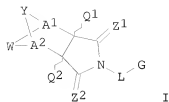
REFERENCE COUNT:

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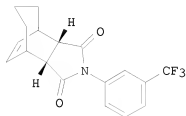
THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 8 CA COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 137:216934 CA
 TITLE: Preparation of fused cyclic succinimide compounds and
 analogs thereof, as modulators of nuclear hormone
 receptor function
 INVENTOR(S): Salvati, Mark E.; Attar, Ricardo M.; Gottardis, Marco
 M.; Balog, James A.; Pickering, Dacia A.; Martinez,
 Rogelio L.; Sun, Chongqing
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
 SOURCE: PCT Int. Appl., 331 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002067939	A1	20020906	WO 2002-US5302	20020220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20040087548	A1	20040506	US 2002-75870	20020214
CA 2439265	A1	20020906	CA 2002-2439265	20020220
AU 2002250163	A1	20020912	AU 2002-250163	20020220
EP 1379249	A1	20040114	EP 2002-719057	20020220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
HU 2003004055	A2	20040428	HU 2003-4055	20020220
JP 2004523558	T	20040805	JP 2002-567306	20020220
US 20060111424	A1	20060525	US 2005-311731	20051219
PRIORITY APPLN. INFO.:			US 2001-271672P	P 20010227
			US 2002-75870	A1 20020214
			WO 2002-US5302	W 20020220
OTHER SOURCE(S):	MARPAT 137:216934			
GI				



I



II

AB Title compds. I [G = (un)substituted cycloalkenyl, aryl or heterocyclo (mono or polycyclic); Z1 and Z2 independently = O, S, NH or substituted amine; L = bond, substituted alkyl chain, NH, substituted amine; A1 and A2 independently = CR1 or N when Y = J-J'-J'' where J = (CR1R1')_n with n = 0-3, J' = bond, carbonyl, CR1R1', R2P:O, R2P:S, etc., and W = CR1R1'-CR1R1', CR3:CR3', (un)substituted cycloalkyl, etc.; or when Y is absent A1 and A2 independently = CR1R1' or NR1; or when Y is absent A1, A2 and W together form -NR1-N:N-; Q1 and Q2 independently = H, (un)substituted alkyl, alkenyl, cycloalkyl, etc.; R1 and R1' independently = H, (un)substituted alkyl, alkenyl, cycloalkyl, cycloalkenyl, amino, halo, CN, etc.; R2 = (un)substituted alkyl, cycloalkyl, cycloalkenyl, heterocyclo, aryl, arylalkyl, etc.; R3 and R3' independently = H, (un)substituted alkyl, alkenyl, CN, halo, nitro, amino, etc.] are prepared and methods of using such compds. in the treatment of nuclear hormone receptor-associated conditions, and pharmaceutical compns. containing such compds

are disclosed. Thus, II was prepared by cyclocondensation of (3α,4β,8β,8α)-4,5,6,7,8,8a-hexahydro-4,8-etheno-1H-cyclohepta[c]furan-1,3(3aH)dione (preparation given) with 3-(trifluoromethyl)aniline. Combinatorial methods of preparing compds. of formula I are also provided. As modulators of nuclear hormone receptor function, the use of I as potential anticancer agents and for treatment of immune disorders is claimed (no data).

IT 455272-94-3P

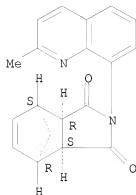
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)
(target compound; preparation of combinatorial libraries of substituted

fused cyclic isoindoleiones as modulators of nuclear hormone receptor function)

RN 455272-94-3 CA

CN 4,7-Methano-1H-isoindole-1,3(2H)-dione,
3a,4,7,7a-tetrahydro-2-(2-methyl-8-quinolinyl)-, (3aR,4S,7R,7aS)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 8 CA COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 136:21013 CA

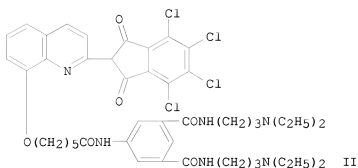
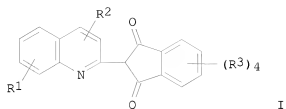
TITLE: Quinophthalone compounds, pigment dispersants therewith, their pigment dispersion compositions and colored photosensitive compositions
 INVENTOR(S): Takeda, Akihiko; Sugiyama, Takekatsu; Kodama, Tomohiro
 PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.
 CODEN: JKXXAF

DOCUMENT TYPE: Patent
 LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
JP 2001335711	A	20011204	JP 2000-159244	20000529
PRIORITY APPLN. INFO.:			JP 2000-159244	20000529
OTHER SOURCE(S):	MARPAT	136:21013		
GI				



AB Title compds. show a structure as I [R1 = Q1Q2 and R2 = H, alkyl; or vice versa, Q1 = divalent group, Q2 = C6H5-a(XYZ)a, X = O, CONH, NHCO, COO, Y = low alkylene, Z = low alkylamino or N-containing 5-6 membered ring, a = 1-2; R3 = H, Cl]. A composition comprising C.I. pigment yellow 138 8.3, II

[prepared

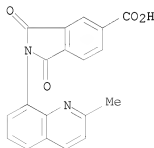
from 8-hydroxy-2-methylquinoline, Et 6-bromohexanoate, bis(3-diethylaminopropylamido) 5-aminoisophthalate, and tetrachlorophthalic anhydride] 0.8, benzyl methacrylate-methacrylic acid copolymer 20.8, and 1-methoxy-2-Pr acetate 50.1 g showed viscosity 15 cP, which was used to prepare a photosensitive composition resulting high contrast value.

IT 377741-57-6P

RL: CRT (Combinatorial reactant); IMF (Industrial manufacture); RCT (Reactant); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant or reagent)
(manufacture of quinophthalone dispersants for pigment dispersion compns. for color filters)

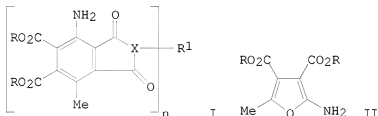
RN 377741-57-6 CA

CN 1H-isoindole-5-carboxylic acid, 2,3-dihydro-2-(2-methyl-8-quinolinyl)-1,3-dioxo- (CA INDEX NAME)



L7 ANSWER 4 OF 8 CA COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 95:97579 CA
 ORIGINAL REFERENCE NO.: 95:16387a,16390a
 TITLE: Substituted anilines
 INVENTOR(S): Schefczik, Ernst
 PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 15 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2924066	A1	19801218	DE 1979-2924066	19790615
PRIORITY APPLN. INFO.: GI			DE 1979-2924066	A 19790615

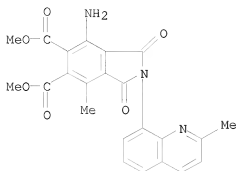


AB The title compds. [I; R = C1-8 alkyl; n = 1, X = O, XR1 = optionally substituted NH; n = 2, X = N, R1 = bond, divalent group] were prepared by the reaction of II with maleic anhydride (III) or a maleimide. Thus, II (R = Me) was heated with III in HOAc to give 94.5% I (R = Me, XR1 = O, n = 1). I are useful as diazo components or fluorescent agents.

IT 77554-64-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 77554-64-4 CA

CN 1H-Isindole-5,6-dicarboxylic acid,
 4-amino-2,3-dihydro-7-methyl-2-(2-methyl-8-quinolinyl)-1,3-dioxo-,
 5,6-dimethyl ester (CA INDEX NAME)



L7 ANSWER 5 OF 8 CA COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 87:7472 CA
 ORIGINAL REFERENCE NO.: 87:1203a,1206a
 TITLE: Coloring of polymers
 INVENTOR(S): Shimada, Keizo; Harada, Toshiaki; Koga, Masahiro
 PATENT ASSIGNEE(S): Teijin, Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

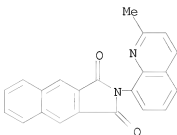
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 51147544	A	19761217	JP 1975-70752	19750613
JP 58012904	B	19830310		
DE 2626271	A1	19761223	DE 1976-2626271	19760611
DE 2626271	B2	19800911		
DE 2626271	C3	19810514		
CA 1078833	A1	19800603	CA 1976-254649	19760611
FR 2314226	A1	19770107	FR 1976-17926	19760614
FR 2314226	B1	19781117		
PRIORITY APPLN. INFO.:			JP 1975-70220	A 19750612
			JP 1975-70221	A 19750612
			JP 1975-70752	A 19750613

GI

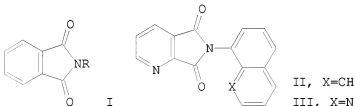
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Plastics and polyester fibers were colored yellow with I (R = Br, Cl; R1, R2 = H, Br) and II (R = H [61975-16-4], Br [61975-18-6]). For example, I (R = Cl, R1 = R2 = H) [61975-13-1] was prepared from 8-(2,3-naphthalenedicarboximido)quinaldine [62783-05-5] and tetrachlorophthalic anhydride [117-08-8] in the presence of ZnCl2, pelletized with polystyrene [9003-53-6] in 0.2:200 ratio at 230°, and injection-molded at 220-80° (dwelling time 2 min) to give a yellow molding with lightfastness rating >6.

IT 62783-05-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with tetrachlorophthalic anhydride)
 RN 62783-05-5 CA
 CN 1H-Benz[*f*]isoindole-1,3(2H)-dione, 2-(2-methyl-8-quinolinyl)- (CA INDEX NAME)

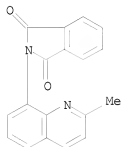


L7 ANSWER 6 OF 8 CA COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 85:42101 CA
 ORIGINAL REFERENCE NO.: 85:6835a,6838a
 TITLE: Negative geotropic effect and phytotoxicity of N-quinolinephthalamic acids and related substances
 AUTHOR(S): Pagani, G.; Caccialanza, G.
 CORPORATE SOURCE: Dep. Chim. Farm., Univ. Pavia, Pavia, Italy
 SOURCE: Farmaco, Edizione Scientifica (1976), 31(5), 364-71
 CODEN: FRPSAX; ISSN: 0430-0920
 DOCUMENT TYPE: Journal
 LANGUAGE: Italian
 GI



AB Eleven N-phthalimidoquinolines I (R = quinolyl, methylquinolyl, methoxyquinolyl, etc.) were prepared and tested for neg. geotropic effect on *Lens esculenta* seedling roots, and for phytotoxic activity on 5 weed species. N-(2-quinolyl)phthalimide [49608-97-1], N-(8-quinolyl)phthalimide [19348-61-9], N-(2-methyl-8-quinolyl)phthalimide [59679-83-3] and N-(6-methoxy-8-quinolyl)phthalimide [59679-84-4] had the highest geotropic effect, which was identical to that of the standard N-(α -naphthyl)phthalimide. The 3 latter compds. showed the highest phytotoxic activity, especially when applied pre-emergence. II [37458-44-9] and III [59679-88-8], pyridine analogs of I, showed little activity.

IT 59679-83-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and herbicidal and geotropic activity of)
 RN 59679-83-3 CA
 CN 1H-Isindole-1,3(2H)-dione, 2-(2-methyl-8-quinolinyl)- (CA INDEX NAME)



L7 ANSWER 7 OF 8 CA COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 54:2349 CA

ORIGINAL REFERENCE NO.: 54:582f-i,583a-c

TITLE: Indenones substituted by quinolyl, pyridyl and benzimidazolyl radicals

INVENTOR(S): Amstutz, Edward D.; Krueger, Geraldine L.

PATENT ASSIGNEE(S): Wm. S. Merrell Co.

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

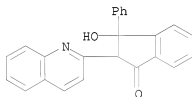
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2894952		19590714	US 1957-683214	19570911

AB Certain 3-(R-substituted)-2-(Y-substituted)-1-indenones were prepared wherein R was a phenyl, lower alkyl phenyl, lower alkoxyphenyl or halophenyl radical and Y was a 2-pyridyl, 2-quinolyl, or 2-benzimidazolyl radical. By lower alkyl and lower alkoxy were meant groups containing 1 to 4 C atoms. Preferred halogens were Cl and Br. These compds. were used in treatment of inflammatory diseases such as rheumatoid arthritis, in the reversal of acute inflammatory lesions such as those of the eye, and for topical application on the skin and mucous membrane as in vaginitis. For oral or parenteral use dosage was 250 mg. to 1 g. daily. They could be a part of creams, ointments or lotions. For example, the intermediate 3-hydroxy-3-phenyl-2-(2-pyridyl)-1-indanone (I), was prepared by adding 0.94 g. Li filings in 50 cc. ether to a solution of 10.52 g. bromobenzene in 13 ml. ether under gentle reflux. After the mixture was cooled, 4.46 g. pyrophthalone was added during 0.5 hr. The solution was stirred 1 hr., refluxed 1 hr., water added and ether distilled during addition of 10% H₂SO₄ (acidification). A yellow solid was filtered off, washed with 10% H₂SO₄ and water and then washed with toluene. Crude product m. 134° (vigorous decomposition); after recrystn. from 95% EtOH it m. 142.2-2.8°. When I was heated until no yellow color remained, a red-orange solid, 3-phenyl-2-(2-pyridyl)-1-indenone (II), resulted. II recrystd. from 50% EtOH-H₂O m. 129.8-30.8°; picrate m. 198-199.4°; oxime m. 185-6.5°. Similarly prepared were: the intermediate, 3-hydroxy-3-(p-methoxyphenyl)-2-(2-pyridyl)-1-indanone (III),

m. 159-60°; orange flakes of 3-(p-methoxyphenyl)-2-(2-pyridyl)-1-indenone (IV), m. 155.5-6.0°; the intermediate, 3-hydroxy-3-(p-tolyl)-2-(2-pyridyl)-1-indanone (V), m. 150-55°; bright red flakes of 3-(p-tolyl)-2-(2-pyridyl)-1-indenone (VI), m. 155-6°; the intermediate, a yellow solid, 3-hydroxy-3-(m-tolyl)-2-(2-pyridyl)-1-indanone (VII), m. 130-45°; an orange solid, 3-(m-tolyl)-2-(2-pyridyl)-1-indenone (VIII), m. 107-10°; the intermediate, a yellow solid, 3-hydroxy-3-(p-chlorophenyl)-2-(2-pyridyl)-1-indanone (IX), m. 150-60°; 3-(p-chlorophenyl)-2-(2-pyridyl)-1-indenone (X), m. 135.5-37.5°; the intermediate 3-hydroxy-3-phenyl-2-(2-quinolyl)-1-indanone (XI), a yellow solid, m. 182°; 3-phenyl-2-(2-quinolyl)-1-indenone-HCl (XII), orange crystals, m. 220-28°; the intermediate, a pale yellow solid, 3-hydroxy-3-phenyl-2-(2-benzimidazolyl)-1-indanone (XIII), m. 235°; 3-phenyl-2-(2-benzimidazolyl)-1-indenone (XIV), dark red, m. 255-57°. Methods were given for preparation of tablets, capsules, injectable suspensions, oral suspensions and ointments. The intermediate III also exhibited anti-inflammatory activity. It was useful orally, parenterally, and topically in dosages and uses described.

IT 102543-48-6P, 1-Indanone, 3-hydroxy-3-phenyl-2-(2-quinolyl)-
 RL: PREP (Preparation)
 (preparation of)
 RN 102543-48-6 CA
 CN 1H-inden-1-one, 2,3-dihydro-3-hydroxy-3-phenyl-2-(2-quinolyl)- (CA
 INDEX NAME)



L7 ANSWER 8 OF 8 CA COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 53:51147 CA
 ORIGINAL REFERENCE NO.: 53:9210h-i,9211a-i,9212a-f
 TITLE: Pyrophthalone and related compounds
 AUTHOR(S): Manly, Donald G.; Richardson, Alfred, Jr.; Stock, Albert M.; Tilford, C. H.; Amstutz, E. D.
 CORPORATE SOURCE: Lehigh Univ., Bethlehem, PA
 SOURCE: Journal of Organic Chemistry (1958), 23, 373-80
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 GI For diagram(s), see printed CA Issue.
 AB Pyrophthalone (I) and other 2-substituted 1,3-indandiones, R2C6H3.CO.CRR1.CO (II), their reaction products with organometallic compds., C6H4.CO.CRR1.CR2OH (III), the carbinol dehydration products, C6H4.CO.CR:CR1 (IV), and some indene, C6H4.CR1R2.CR:COH (V) and indan reduction products were prepared. Chemical evidence and infrared spectra comparison showed that I and some II exist in a chelated enol form. Various methods were investigated but most II were synthesized by condensing (o-C6H4CO)2 (VI) with an alkyl heterocycle. Von Huber

[Ber. 36, 1653(1903)] heated equimolar VI and an active Me compound 5 hrs. at 200° with a catalytic amount of ZnCl₂ (method A). The same procedure was used with 2 moles active Me compound in a sealed tube (method B). In the procedure of Ogilvie (U.S. 1,963,374, C.A. 28, 52519) the reactants and catalyst in PhNO₂ were refluxed 6 hrs., the cooled mixture filtered, and the Et₂O-washed residue recrystd. (EtNO₂, PhNO₂, or EtOH) (method C). In method D, o-C₆H₄(COCl)₂ in C₆H₆ was used in place of VI. Method E used H₃PO₄ as catalyst. The phthalone in AcOH treated dropwise with 0.5 mole Br, the stirring continued 10 min., the mixture filtered and the residue slurried in H₂O, the slurry made slightly basic with 5% NaOH, and the filtered residue washed and dried gave II according to method F. VI (1 mole) and 1 mole 2-methyl-benzimidazole was heated 2 hrs. at 200° according to van Alphen (C.A. 34, 50805), the product washed (hot water and AcOH) until the washings were clear, the product taken up in concentrated H₂SO₄, and reprecipitated with H₂O (method G). The reactive

H atoms were usually restricted to those in a Me group and the most reactive groups were those adjacent to the heterocyclic N. No product was formed by reaction of 2 Me groups. The methods of synthesis and physical data are tabulated for II (R, R₁, R₂, method of preparation, % yield, and m.p. given): 2-C₅H₄N, H, H (I), A, 7.2, 289-91°, B, 39.9, 290-2°, C, 43.1, 285-90°, D, 18, 287-90°, E, 28, 288-91°; 6,2-MeC₅H₃N, H, H, C, 12, 218-19°; 5,2-EtC₅H₃N, H, H, A, 31, 235-7°, C, 21, 235-7°; 2-C₅H₄N, Br, H, F, -, 152-4°; 3,2-MeC₅H₃N, H, H, C, 2.1, 178-80°; 4,2-MeC₅H₃N, H, H, C, 11, 259-60°; 2-C₅H₄N, Me, H, D, 15, 137-8°; 2-C₅H₄N, H, 4-NO₂, C, 3.2, 315-16°; 6,2-MeC₅H₃N, H, 4-NO₂, A, 14, 293-4°; 2-C₅H₄N, H, 5-NO₂, A, 17, 352-5°; 2-C₅H₄N, Ph, H (VII), D, 52, 152-3°; 2-C₅H₅N, H, H (VIII), C, 42, 241-2°; 2-benzothiazolyl, H, H (IX), A, 51, 350-60°; 2-(5-chlorobenzimidazolyl), H, H (X), C, 61, above 480°; 2-benzimidazolyl, H, H (XI), G, 67, above 500°. Little success was had in the preparation of N-substituted pyrophthalones. For reduction of II, organolithium compds. were prepared from the appropriate halide with a molar ratio of 4:2:1 Li-organic halide-II. Finely divided Li in 35 parts by weight absolute Et₂O was stirred under gentle reflux with controlled addition of 0.5M halide in Et₂O, the mixture gently refluxed with controlled addition of finely powdered II, stirred under reflux to neg. Gilman test, chilled (ice-bath) and stirred with slow addition of an equal volume of dilute aqueous NH₄Cl, the mixture

stirred 30 min. and filtered, the solid III washed with water, and dried (method H). PhCH₂MgCl (4 moles) prepared according to Gilman and Meyers [Organic Syntheses 4, 59(1925)] was refluxed 1 hr. with addition of 1 mole II and the mixture worked up as in method H (method I). III dehydrated readily and purification for characterization was difficult. Methods and data for III are tabulated (reactant, R, R₁, R₂, method of preparation, % yield, and m.p. given): I, 2-C₅H₄N, H, Ph (XII), H, 80, 142-3°; I, 2-C₅H₄N, H, p-MeOC₆H₄ (XIII), H, 70, 156-7°; I, 2-C₅H₄N, H, p-MeC₆H₄ (XIV), H, 92, 150°; I, 2-C₅H₄N, H, m-MeC₆H₄ (XV), H, 75, 130°; I, 2-C₅H₄N, H, o-MeC₆H₄ (XVI), H, 70, 145-55°; I, 2-C₅H₄N, H, p-ClC₆H₄ (XVII), H, 80, 150-60°; VIII, 2-C₉H₆N, H, Ph (XVIII), H, 100, 164°; IX, 2-benzothiazolyl, H, Ph (XIX), H, 89, above 360°; X, 2-(5-chlorobenzimidazolyl), H, Ph, H, 49, above 510°; I, 2-C₅H₄N, H, PhCH₂ (XX), I, 68, 100-20°; XI, 2-benzimidazolyl, H, Ph (XXI), J, 94, 235°. Also prepared were (reactant, product, method, % yield, and m.p. given): 2-indanone, 2-(2-pyridyl)-2-indanol, H, 10, 119-20°; 1-indanone,

1-(2-pyridyl)-1-indanol, H, 33, 78-80°;
 3-phenyl-2-(2-pyridyl)indenone (XXII),
 1,3-diphenyl-2-(2-pyridyl)1-inden-3-ol (XXIII), H (the phthalone in C6H6 added to PhLi in Et2O, the mixture treated with dilute HCl and the product crystallized from HCl), 78, 237-8°; VII,
 1,2,3-triphenyl-2-(2-pyridyl)-1,3-indandiol (XXIV), H, 90, 107°.
 In the reaction with XXII and VII a 2nd mole of PhLi added with formation of XXIII and XXIV. The dried III prepared by method H or I were either heated above the m.p. until effervescence ceased and the uniformly colored melt recrystd. (method J) or taken up in concentrated HCl with effervescence, the red solution stirred 15 min. at 0°, neutralized with aqueous NaOH, the compound, washed (10% aqueous NaHCO3) and the dried material crystallized (method K)

to give the indenones IV (reactant, R, R1, method, % yield, and m.p. given): XII, 2-C5H4N, Ph, J, 100, 130-1°, K, 82, 129-31°;
 XIII, 2-C5H4N, p-MeOC6H4 (XXV), J, 100, 155-6°; XIV, 2-C5H4N, p-MeC6H4 (XXVI), J, 100, 155-6°; XV, 2-C5H4N, m-MeC6H4 (XXVII), J, 100, 107-10°; XVI, 2-C5H4N, o-MeC6H4, J, 100, 121-2°; XVII, 2-C5H4N, p-ClC6H4 (XXVIII), J, 100, 136-8°;
 XVIII, 2-C9H6N, Ph (XXIX), K, 96, 220°; XIX, 2-benzothiazolyl, Ph (XXX), K, 100, 169-70°; XX, 2-C5H4N, PhCH2, K, 54, 65-100° (gum); XXI, 2-benzimidazolyl, Ph, K, 100, 255-7°. III and IV were unable to enolize to form chelates so that picrates, oximes, and occasionally 2,4-dinitrophenylhydrazones were obtained. Reductions were carried out catalytically with PtO2 or Raney Ni catalysts (method L), according to Clemmensen (method M), and with NaBH4 (method N). Vigorous catalytic hydrogenation not only reduced indene double bonds but occasionally reduced part or all of the heterocyclic ring substituent. XXII (5.7 g.) in 250 absolute alc. hydrogenated 78 hrs. at 2 atmospheric with

0.2 g.

Raney Ni W-6 gave 60% V (R = 2-C5H4N, R1 = H, R2 = Ph) (XXXI), m. 188-9°. XXII (10 g.) in 30 ml. dioxane hydrogenated 16 hrs. at 2 atmospheric with 2.0 g. Raney Ni gave 10% alc.-insol. product, m. 148-9°, and 30% XXXI, also produced in 49% yield by method N. Similar reductions gave V (reactant, R, R1, R2, method, % yield, and m.p. given): XXII, 2-(3,4,5,6-tetrahydropyridyl), H, Ph, L, 46, 212-13°; XXIX, 2-(3,4-dihydroquinolyl), H, Ph, N, 86°, 275°; IX, 2-benzothiazolyl, H, HO, N, 100, 345-8°; XXX, 2-benzothiazolyl, H, Ph, N, 50, 151-2°; XXVI, 2-dihydropyridyl, H, p-MeC6H4, N, 43, 183-4°. VII (1 mole), 598 g. mossy Zn, 47.9 g. HgCl2, 30 ml. concentrated HCl, and 720 ml. H2O shaken vigorously 10 min., the residue after decanting treated with 450 ml. H2O, 598 ml. concentrated HCl, and 1 mole VII, the oily mixture treated with 450 ml. H2O and 598 ml. concentrated HCl, the

mixture

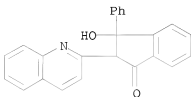
treated 5 times at hourly intervals with 59.8 ml. concentrated HCl and refluxed 17 hrs., the cooled solution filtered, the residue basified with NaOH, and the water-washed product recrystd. (alc. or EtNO2) yielded 60% 2-phenyl-2-(2-pyridyl)-3-indan-1-ol, m. 186-7°. XXII was not reduced by method M. XXII (3.3 g.) in 30 ml. absolute alc. containing 3 molar equivs. dry HCl hydrogenated 24 hrs. at 2100 lb./sq. in. with 20 mg. PtO2 gave 15% 3-phenyl-2-(2-piperidyl)-1,3-indandiol, m. 135-6°. I (6 g.) in 50 ml. MeOH and 2.7 ml. concentrated HCl hydrogenated at 60 lb./sq. in. over 0.5 g. PtO2 gave 11% 2-(2-piperidyl)-1,3-indandiol; HCl salt, m. 230-2° (decomposition). VII (2 g.) in 50 ml 80% AcOH hydrogenated over PtO2 yielded 8% 2-phenyl-2-(2-piperidyl)-1,3-indandiol, m. 184-6°; 2 hrs. hydrogenation of 7.5 g. I in 100 ml. AcOH over 0.8 g. PtO2 gave 41% 2-(2-piperidyl)-1,3-hexahydroindandiol. Extensive pharmacol. screening

showed 6 indenones, XXII, XXV, XXVI, XXVII, XXVIII, XXIX, and the carbinol XIII, precursor to the indenone XXV, to have antiarthritic activity.

IT 102543-48-6P, 1-Indanone, 3-hydroxy-3-phenyl-2-(2-quinolyl)-
 RL: PREP (Preparation)
 (preparation of)

RN 102543-48-6 CA

CN 1H-Inden-1-one, 2,3-dihydro-3-hydroxy-3-phenyl-2-(2-quinolyl)- (CA
 INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 10:02:19 ON 11 FEB 2009)

FILE 'REGISTRY' ENTERED AT 10:02:26 ON 11 FEB 2009

L1 STRUCTURE UPLOADED
 L2 STRUCTURE UPLOADED
 L3 0 S L1 SAM
 L4 0 S L2 SAM
 L5 2 S L1 FULL
 L6 12 S L2 FULL

FILE 'CA' ENTERED AT 10:03:43 ON 11 FEB 2009

L7 8 S L5 OR L6

=> s organic pigment crystal?

411338 ORGANIC
 161921 PIGMENT
 1956108 CRYSTAL?

L8 2 ORGANIC PIGMENT CRYSTAL?
 (ORGANIC(W)PIGMENT(W)CRYSTAL?)

=> d kwic

L8 ANSWER 1 OF 2 CA COPYRIGHT 2009 ACS on STN

TI Manufacture of organic pigment crystals with
 high purity and good controllability of crystal structures

=> d 2 kwic

L8 ANSWER 2 OF 2 CA COPYRIGHT 2009 ACS on STN

TI Fractal analysis of organic pigment crystals

=> s pigment cryst? proce?

161921 PIGMENT

2272187 CRYST?
 4981145 PROCE?
 L9 0 PIGMENT CRYST? PROCE?
 (PIGMENT(W)CRYST?(W)PROCE?)

=> s pigment cryst?
 161921 PIGMENT
 2272187 CRYST?
 L10 289 PIGMENT CRYST?
 (PIGMENT(W)CRYST?)

=> d l8 ibib abs

L8 ANSWER 1 OF 2 CA COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 139:8131 CA
 TITLE: Manufacture of organic pigment
 crystals with high purity and good
 controllability of crystal structures
 INVENTOR(S): Mizuguchi, Hitoshi
 PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003160738	A	20030606	JP 2001-362469	20011128
PRIORITY APPLN. INFO.:			JP 2001-362469	20011128

AB The manufacturing method contains heat-dissolving organic pigments in solvents under pressure and slowly cooling for crystallization. Thus, titanyle phthalocyanine, 1-chloronaphthalene, and H₂O were sealed in a reactor, heated at 180° for 10 min, and cooled to 60° at a rate of 3°/h to give crystals with dimensions of 200 + 400 + 150 μm. The pigments are useful for electroluminescence devices, electrophotog. toners, etc.

=> d his

(FILE 'HOME' ENTERED AT 10:02:19 ON 11 FEB 2009)

FILE 'REGISTRY' ENTERED AT 10:02:26 ON 11 FEB 2009

L1 STRUCTURE UPLOADED
 L2 STRUCTURE UPLOADED
 L3 0 S L1 SAM
 L4 0 S L2 SAM
 L5 2 S L1 FULL
 L6 12 S L2 FULL

FILE 'CA' ENTERED AT 10:03:43 ON 11 FEB 2009

L7 8 S L5 OR L6
 L8 2 S ORGANIC PIGMENT CRYSTAL?
 L9 0 S PIGMENT CRYST? PROCE?
 L10 289 S PIGMENT CRYST?

10/560039

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---Logging off of STN---

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Executing the logoff script...

=> LOG Y

STN INTERNATIONAL LOGOFF AT 10:06:18 ON 11 FEB 2009